

Salicylic acid
69-72-7 | DTXSID7026368

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.81	0.55	0.81	0.54	0.71	0.61

Model Results

Predicted value: 50.6 L/kg

Global applicability domain: Inside

Local applicability domain index: 6.96e-01

Confidence level: 6.43e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>4-Aminobenzoic acid</div> <div>Measured: 316</div> <div>Predicted: 96.6</div>	<div>Image not found</div> <div>(2-Fluorophenyl)urea</div> <div>Measured: 20.9</div> <div>Predicted: 52.8</div>	<div>Image not found</div> <div>Urea, (m-fluorophenyl)-</div> <div>Measured: 58.9</div> <div>Predicted: 59.1</div>
<div>Image not found</div> <div>6-Chloro-2-picolinic acid</div> <div>Measured: 23.4</div> <div>Predicted: 53.1</div>	<div>Image not found</div> <div>1-Phenylurea</div> <div>Measured: 22.4</div> <div>Predicted: 34.2</div>	